Electronic Supplementary Information (ESI) for

Handedness inversion of the self-assemblies of lipotetrapeptides regulated by the shift of methyl group

Kexiao Guo, Wei Liu*, Yong Wang, He Wei, Baozong Li, Yi Li* and Yonggang Yang*

State and Local Joint Engineering Laboratory for Novel Functional Polymeric Materials, Jiangsu Key Laboratory of Advanced Functional Polymer Design and Application, Jiangsu Engineering Laboratory of Novel Functional Polymeric Materials, Department of Polymer Science and Engineering, College of Chemistry, Chemical Engineering and Materials Science, Key Laboratory of Polymeric Materials Design and Synthesis for Biomedical Function, Soochow University, Suzhou 215123, China.
Email: W. Liu, weiliu@suda.edu.cn; Y. Li, liyi@suda.edu.cn; Y. Yang. ygyang@suda.edu.cn.

Table S1 MGCs of the lipotetrapeptides in organic solvents.

	11GGGA	11GGAG	11GAGG	11AGGG
DMF	Solution	Solution	Solution	Solution
DMSO	Solution	Solution	Solution	Solution
THF	Insoluble	Insoluble	Insoluble	Insoluble
Acetone	Insoluble	Insoluble	Insoluble	Insoluble
Toluene	Insoluble	Insoluble	Insoluble	Insoluble
Acetonitrile	Insoluble	Insoluble	Insoluble	Insoluble
n-Hexane	Insoluble	Insoluble	Insoluble	Insoluble
Ethyl acetate	Insoluble	Insoluble	Insoluble	Insoluble
1,4-Dioxane	Insoluble	Insoluble	Insoluble	Insoluble
MeOH/Water	10 (6/4, v/v)	10 (5/5, v/v)	10 (4/6, v/v)	Precipitate
DMSO/H_2O	10 (6/4, v/v)	10 (6/4, v/v)	10 (6/4, v/v)	10 (6/4, v/v)

The data shown in the above table refer to the minimum gelation concentrations (MGCs) (g L^{-1}) of the lipotetrapeptides in the listed organic solvents at 25^oC. Solution: no gelation occurred at a concentration of 30 g L^{-1}.
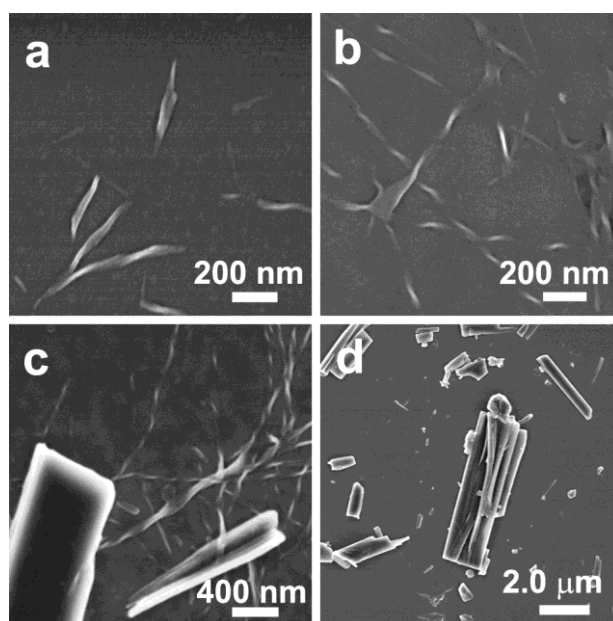

Fig. S1 FE-SEM images of 11AGGG self-assemblies taken after different aging times.
(a) 2 min; (b) 6 min; (c) 8 min; (d) 15 min.

Computation details

The molecular optimization for the compounds were carried out with Gaussian 09 programs,[S1] and density functional theory (DFT) with thethree-parameter hybrid functional (B3LYP) were employed.[S2] A 6-31G* basis set was used for all atoms.

References

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